10556229

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| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | NOV 21 | CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present |
| NEWS 3 | NOV 26 | MARPAT enhanced with FSORT command |
| NEWS 4 | NOV 26 | CHEMSAFE now available on STN Easy |
| NEWS 5 | NOV 26 | Two new SET commands increase convenience of STN searching |
| NEWS 6 | DEC 01 | ChemPort single article sales feature unavailable |
| NEWS 7 | DEC 12 | GBFULL now offers single source for full-text coverage of complete UK patent families |
| NEWS 8 | DEC 17 | Fifty-one pharmaceutical ingredients added to PS |
| NEWS 9 | JAN 06 | The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo |
| NEWS 10 | JAN 07 | WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data |
| NEWS 11 | FEB 02 | Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE |
| NEWS 12 | FEB 02 | GENBANK enhanced with SET PLURALS and SET SPELLING |
| NEWS 13 | FEB 06 | Patent sequence location (PSL) data added to USGENE |
| NEWS 14 | FEB 10 | COMPENDEX reloaded and enhanced |
| NEWS 15 | FEB 11 | WTEXTILES reloaded and enhanced |
| NEWS 16 | FEB 19 | New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art |
| NEWS 17 | FEB 19 | Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01 |
| NEWS 18 | FEB 23 | Several formats for image display and print options discontinued in USPATFULL and USPAT2 |
| NEWS 19 | FEB 23 | MEDLINE now offers more precise author group fields and 2009 MeSH terms |
| NEWS 20 | FEB 23 | TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms |
| NEWS 21 | FEB 23 | Three million new patent records blast AEROSPACE into STN patent clusters |
| NEWS 22 | FEB 25 | USGENE enhanced with patent family and legal status display data from INPADOCDB |
| NEWS 23 | MAR 06 | INPADOCDB and INPAFAMDB enhanced with new display formats |
| NEWS 24 | MAR 11 | EPFULL backfile enhanced with additional full-text applications and grants |

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 NEWS 25  MAR 11  ESBIOBASE reloaded and enhanced
 NEWS 26  MAR 20  CAS databases on STN enhanced with new super role
                  for nanomaterial substances
 NEWS 27  MAR 23  CA/CAplus enhanced with more than 250,000 patent
                  equivalents from China

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:27:04 ON 25 MAR 2009

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.22       0.22

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STRUCTURE FILE UPDATES:   23 MAR 2009  HIGHEST RN 1125796-38-4
DICTIONARY FILE UPDATES:  23 MAR 2009  HIGHEST RN 1125796-38-4

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http://www.cas.org/support/stngen/stndoc/properties.html

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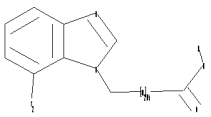
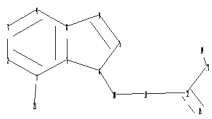




chain nodes :
10 11 12 13 14 15 21
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-21 6-10 10-11 11-12 12-13 12-15 13-14
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
1-21 5-6 5-9 6-7 6-10 8-9 12-13 12-15
exact bonds :
10-11 11-12 13-14
normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

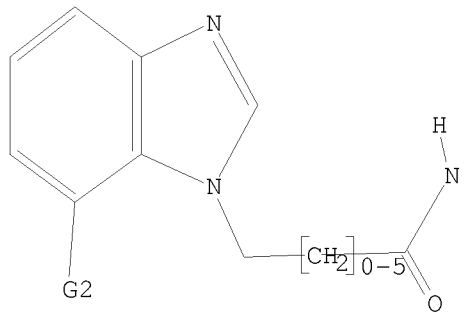
G1:H,Ak,CH3

G2:X,Ak,CN,NH2,NO2,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 21:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR




G1 H,Ak,Me

G2 X,Ak,CN,NH2,NO2,Hy

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 10:27:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2846 TO ITERATE

70.3% PROCESSED 2000 ITERATIONS 18 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 53720 TO 60120
PROJECTED ANSWERS: 209 TO 815

L2 18 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:27:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 56286 TO ITERATE

100.0% PROCESSED 56286 ITERATIONS 361 ANSWERS

SEARCH TIME: 00.00.04

L3 361 SEA SSS FUL L1

=> FIL HCAPLUS

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 185.88 | 186.10 |

FILE 'HCAPLUS' ENTERED AT 10:27:51 ON 25 MAR 2009
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FILE COVERS 1907 - 25 Mar 2009 VOL 150 ISS 13
FILE LAST UPDATED: 24 Mar 2009 (20090324/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 15 L3

=> s l4 and py<=2003
24034884 PY<=2003
L5 4 L4 AND PY<=2003

=> d l5 ibib abs hitstr tot

L5 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:219222 HCAPLUS
DOCUMENT NUMBER: 132:222537
TITLE: Preparation of substituted nitrogen-containing heterocyclic compounds
INVENTOR(S): Horvath, Andras; Salamon, Zoltan
PATENT ASSIGNEE(S): Hung.
SOURCE: Hung. Teljes, 21 pp.
CODEN: HUXXBU
DOCUMENT TYPE: Patent

LANGUAGE: Hungarian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| HU 78019 | A2 | 19990528 | HU 1995-962 | 19950331 <-- |

PRIORITY APPLN. INFO.: HU 1995-962 19950331
OTHER SOURCE(S): MARPAT 132:222537
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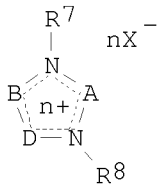
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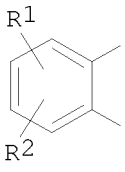
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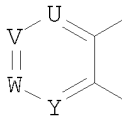
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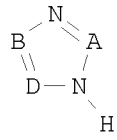
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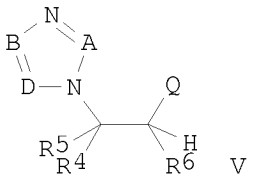
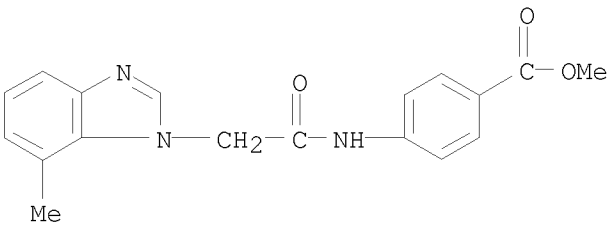

V

AB The title compds. [I; A = CR1, CR3; B = CR1; D = CR2, CR2:CR3, N; BD = II, III; R1-R3 = H, alkyl; U, V, W, Y, Z = (un)substituted Ph, NHCOalkyl, CO2alkyl, etc.; n = 0-1; X = Cl, Br, I, etc.; R7 = H, alkyl, heteroaryl; R8 = H, CR4R5CHR6Q; R4-R6 = H, alkyl, cycloalkyl, Q; Q = CN, CO2alkyl, COalkyl, etc.], useful as intermediates for biol. active compds., were prepared by reacting compound IV with olefin R4R5C:CR6Q followed by treatment of N-monoalkylated compound V with R7X.

IT 172839-71-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted nitrogen-containing heterocyclic compds.)

RN 172839-71-3 HCAPLUS

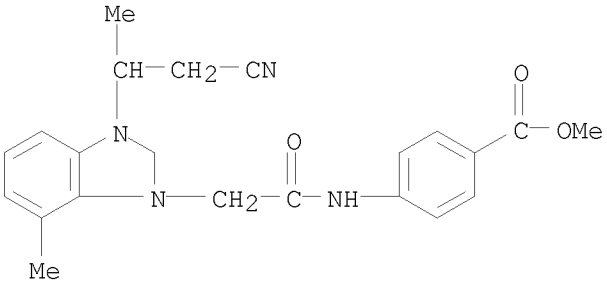
CN Benzoic acid, 4-[[2-(7-methyl-1H-benzimidazol-1-yl)acetyl]amino]-, methyl ester (CA INDEX NAME)



L5 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:866656 HCAPLUS
DOCUMENT NUMBER: 124:117179
ORIGINAL REFERENCE NO.: 124:21829a,21832a
TITLE: Michael adducts in the regioselective synthesis of N-substituted azoles
AUTHOR(S): Horvath, Andras
CORPORATE SOURCE: Alkaloida Chem. Co. Ltd., Tiszavasvari, Hung.
SOURCE: Synthesis (1995), (9), 1183-9
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:117179

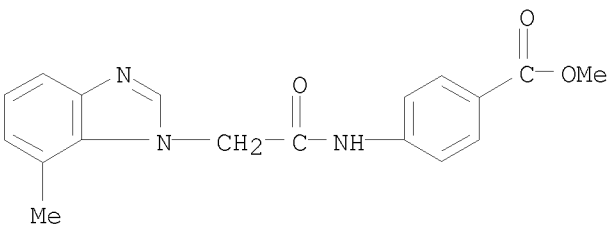
AB Michael adducts of azoles (4-phenyl-, 4-methyl-, and 4-nitroimidazole, 4-methylbenzimidazole, 1,2,4-triazole, and theophylline) are shown to be valuable substrates for obtaining the N-substituted derivs. of the parent heterocycles by a quaternization-Hofmann elimination sequence. The effectiveness of the procedure is dependent on the regiochem. outcome of the 1st, N-protective step, i.e. the Michael addition By choosing the appropriate Michael acceptor, alkylating agent, and deprotection conditions, the thermodynamically less stable regioisomers of N-substituted azoles were obtained in high yields.

IT 172839-61-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-substituted azoles via regioselective Michael addition)
RN 172839-61-1 HCAPLUS
CN 1H-Benzimidazolium, 3-(2-cyano-1-methylethyl)-1-[2-[[4-(methoxycarbonyl)phenyl]amino]-2-oxoethyl]-7-methyl-, bromide (1:1) (CA INDEX NAME)




ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

IT 172839-71-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation via regioselective Michael addition)
RN 172839-71-3 HCAPLUS
CN Benzoic acid, 4-[[2-(7-methyl-1H-benzimidazol-1-yl)acetyl]amino]-, methyl ester (CA INDEX NAME)



L5 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:510007 HCAPLUS
DOCUMENT NUMBER: 97:110007
ORIGINAL REFERENCE NO.: 97:18305a,18308a
TITLE: Benzimidazoles
INVENTOR(S): Jemison, Robert William; Beames, David John
PATENT ASSIGNEE(S): ICI Australia Ltd. , Australia
SOURCE: Pat. Specif. (Aust.), 56 pp.
CODEN: ALXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| AU 519236 | B2 | 19811119 | AU 1978-35043 | 19770422 <-- |
| AU 7835043 | A | 19791018 | | |

PRIORITY APPLN. INFO.: AU 1977-9860 A 19770422
OTHER SOURCE(S): CASREACT 97:110007
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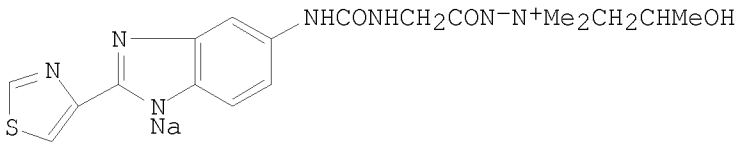
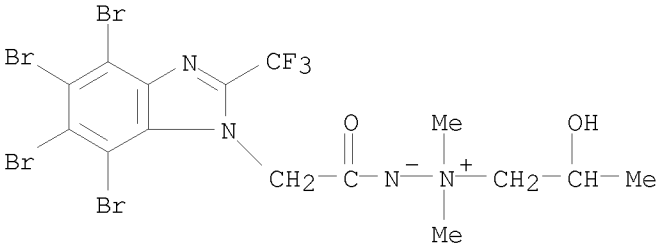


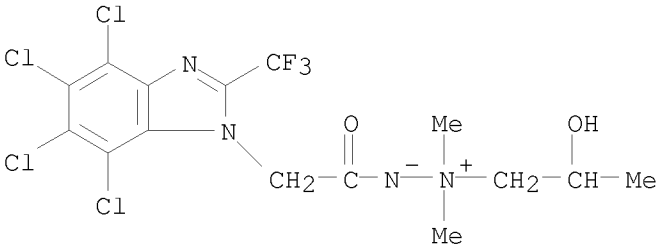
I

AB R[XN-N+R1R2R3]n [R = (un)substituted benzimidazolyl, R1-R3 = (un)substituted alkyl; X = CO, O2C, NHCO, X1CO, COX1CO, NHCOX1CO, CONHX1CO, SO2, 4-SC6H4O2C, NHCONHX1CO, 4-COC6H4O2C, 4-COC6H4NHCO, 4-SOC6H4CO, 4-COC6H4CO, 4-SOC6H4O2C; X1 = alkylene; n = 1-3] were prepared Thus 5-amino-2-(4-thiazolyl)benzimidazole was treated with OCNCH2CO2Me to give the 5-methoxycarbonylmethylureidobenzimidazole derivative which was treated with Me2NNH2 and propylene oxide to give I. At 50 mg/kg s.c. in sheep I reduced the fecal Hemonchus egg count from 800 to 0 on the 2nd day.
IT 82792-01-6P 82792-02-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82792-01-6 HCAPLUS

CN Hydrazinium, 1-(2-hydroxypropyl)-1,1-dimethyl-2-[2-[4,5,6,7-tetrabromo-2-(trifluoromethyl)-1H-benzimidazol-1-yl]acetyl]-, inner salt (CA INDEX NAME)



RN 82792-02-7 HCAPLUS
CN Hydrazinium, 1-(2-hydroxypropyl)-1,1-dimethyl-2-[2-[4,5,6,7-tetrachloro-2-(trifluoromethyl)-1H-benzimidazol-1-yl]acetyl]-, inner salt (CA INDEX NAME)



L5 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:88247 HCAPLUS
DOCUMENT NUMBER: 70:88247
ORIGINAL REFERENCE NO.: 70:16521a,16524a
TITLE: Participation of the anilino group in peptide bond cleavage. Use of tert-butyl 3,5-dinitro-2-fluorocarbanilate as a peptide reagent
AUTHOR(S): Kirk, Kenneth L.; Cohen, Louis A.
CORPORATE SOURCE: Nat. Inst. of Allergy and Metab. Diseases, Nat. Inst. of Health, Bethesda, MD, USA
SOURCE: Journal of Organic Chemistry (1969), 34(2), 395-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Picramyl fluoride (3,5-dinitro-2-fluoroaniline) (I) was prepared by the SnCl2 reduction of picryl fluoride and by the Curtius rearrangement of 3,5-dinitro-2-fluorobenzoyl azide. Reaction of I with peptides (at pH 8) results in replacement of the F atom by the peptide N. Coupling is followed by rapid intramol. attack of the anilino group on the neighboring peptide bond (even at pH 8), resulting in cleavage of that bond and the formation of a dihydro-quinoxalinone derivative of the N-terminal amino acid. By use of I tert-BuO2C derivative, the coupling and cleavage steps can be

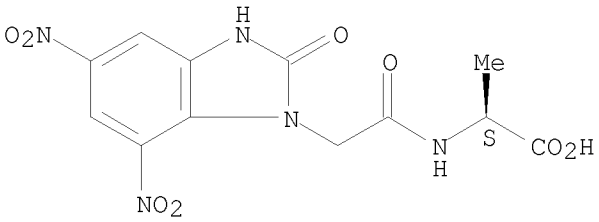
separated Removal of the blocking group by F3CCO2H is followed by rapid cyclization, both reactions proceeding quant. Sequencing of a polypeptide (e.g., oxidized insulin A chain) provides steadily decreasing yields of N-terminal derivs., due to benzimidazolinone formation during the coupling step. By kinetic anal., it is shown that the benzimidazolinone arises from attack of the 2,4-dinitroaniline anion on the adjacent tert-Bu carbanilate group.

IT 18646-10-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18646-10-1 HCAPLUS

CN Alanine, N-[(5,7-dinitro-2-oxo-1-benzimidazolinyl)acetyl]-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d l4 ibib abs tot

L4 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1372392 HCAPLUS

DOCUMENT NUMBER: 150:269

TITLE: Potent benzimidazolone-based CGRP receptor antagonists

AUTHOR(S): Theberge, Cory R.; Bednar, Rodney A.; Bell, Ian M.; Corcoran, Halea A.; Fay, John F.; Hershey, James C.; Johnston, Victor K.; Kane, Stefanie A.; Mosser, Scott; Salvatore, Christopher A.; Williams, Theresa M.; Zartman, C. Blair; Zhang, Xu-Fang; Graham, Samuel L.; Vacca, Joseph P.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck & Co., Inc., West Point, PA, 19486, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(23), 6122-6125
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The previously disclosed spirohydantoin-based CGRP receptor antagonists were optimized for potency through modification of the benzimidazolone substituents. Compds. were identified which had minimal shift in the cAMP functional assay containing 50% human serum. Blockade of CGRP-mediated vasodilation was observed with these compds. in a rhesus pharmacodynamic assay and the in vivo potency correlated with the in vitro activity in the serum-shifted functional assay.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:192495 HCAPLUS
DOCUMENT NUMBER: 148:239209
TITLE: Benzimidazole derivatives as vanilloid receptor antagonists, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Brown, William; Johnstone, Shawn; Labrecque, Denis
PATENT ASSIGNEE(S): AstraZeneca AB, Swed.
SOURCE: PCT Int. Appl., 136pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| WO 2008018827 | A1 | 20080214 | WO 2007-SE720 | | 20070810 |
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| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| US 20080221188 | A1 | 20080911 | US 2007-836221 | | 20070809 |
| AU 2007282186 | A1 | 20080214 | AU 2007-282186 | | 20070810 |
| PRIORITY APPLN. INFO.: | | | US 2006-837249P | P | 20060811 |
| | | | WO 2007-SE720 | W | 20070810 |

OTHER SOURCE(S): MARPAT 148:239209
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention provides benzimidazole derivs. of formula I, which are antagonists of vanilloid receptor 1 (VR-1). In compds. I, R1 is halo, cyano, or acetyl; R2 is H or Me; R3 is H or halo; R4 and R5 are independently selected from Me and Et, or R4 and R5, together with the carbon atom to which they are attached, form C3-6 cycloalkyl or a 5- or 6-membered heterocyclyl; n is 0-2; and each R6 is independently selected from halo, Me, and Et. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound according to formula I and a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment of disorders responding to VR-1 inhibition, such as osteoarthritis, chronic tendinitis, pelvic pain, peripheral neuropathy, gastroesophageal reflux disease, irritable bowel syndrome, and overactive bladder. Substitution of 1,2,3-trifluoro-4-nitrobenzene with ethanolamine followed by hydrogenation, heterocyclization with formic acid, and oxidation

gave benzimidazole II. Double α-methylation of (4-bromophenyl)acetonitrile followed by lithiation, condensation with N-methoxy-N-methyl-acetamide, and reductive amination resulted in the formation of amine III, which underwent amidation with II and chiral HPLC separation to give IV and its enantiomer. Some compds. of the invention express antagonist activity to VR-1 below 100 nM (no specific data).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1177157 HCAPLUS
DOCUMENT NUMBER: 147:448786
TITLE: Preparation of oxadiazole compounds as S1P1 agonists
INVENTOR(S): Harada, Hironori; Hattori, Kazuyuki; Fujita, Kazuya; Morita, Masataka; Imada, Sunao; Abe, Yoshito; Itani, Hiromichi; Morokata, Tatsuaki; Tsutsumi, Hideo
PATENT ASSIGNEE(S): Astellas Pharma Inc., Japan
SOURCE: PCT Int. Appl., 105pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| WO 2007116866 | A1 | 20071018 | WO 2007-JP57414 | | 20070402 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW | | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | | |
| AU 2007236707 | A1 | 20071018 | AU 2007-236707 | | 20070402 |
| CA 2648303 | A1 | 20071018 | CA 2007-2648303 | | 20070402 |
| EP 2003132 | A1 | 20081217 | EP 2007-740850 | | 20070402 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR | | | | | |
| US 20090076070 | A1 | 20090319 | US 2008-244102 | | 20081002 |
| NO 2008004618 | A | 20081217 | NO 2008-4618 | | 20081031 |
| KR 2009007740 | A | 20090120 | KR 2008-726792 | | 20081031 |
| PRIORITY APPLN. INFO.: | | | JP 2006-102544 | A | 20060403 |
| | | | JP 2006-276693 | A | 20061010 |
| | | | JP 2006-279227 | A | 20061012 |
| | | | WO 2007-JP57414 | W | 20070402 |

OTHER SOURCE(S): MARPAT 147:448786
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [ring A = Q1, etc.; X = single bond, -CH2-, -NR3-, etc.; R1 = -H, halo, aryl, etc.; R2 = -CN, -O-alkyl, -CHO, etc.; R3 = -H; R3 and R1, together with the nitrogen to which they are attached, may form morpholino, 1-pyrrolidinyl or 3,4-dihydropiperidin-1-yl (sic); when X is a single bond, R1 and R2 may combine to form a 5-membered ring (wherein 5-membered ring is optionally substituted with alkyl); R4 = Q2, etc. (one bond from Q2 is linked to oxadiazolyl ring); R5 = -H, -CN, -NHRx, etc.; Rx = -H, -OH, (un)protected amino, etc.] or their pharmaceutically acceptable salts were prepared For example, reaction of 1,3-difluoropropan-2-ol with NaH followed by in-situ treatment with 2-[4-[5-(3-chloro-4-fluorophenyl)-1,2,4-oxadiazol-3-yl]-1H-indol-1-yl]acetamide afforded compound II. The exemplified compound II showed the S1P1 agonistic activity with EC50 = 1.2 nM. Compds. I are claimed useful for the treatment of autoimmune disease, multiple sclerosis, etc.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1146647 HCAPLUS

DOCUMENT NUMBER: 147:448636

TITLE: Preparation of indoles, indazoles, benzimidazoles and their analogs as chemokine receptor CXCR4 and CCR7 inhibitors

INVENTOR(S): Thomas, William D.; Leleti, Manmohan Reddy; Pennell, Andrew M. K.

PATENT ASSIGNEE(S): Chemocentryx, Inc., USA

SOURCE: PCT Int. Appl., 142pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2007115231 | A2 | 20071011 | WO 2007-US65729 | 20070330 |
| WO 2007115231 | A3 | 20080717 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA | | | | |
| US 20070275965 | A1 | 20071129 | US 2007-731695 | 20070330 |

PRIORITY APPLN. INFO.: US 2006-787925P P 20060330

OTHER SOURCE(S): MARPAT 147:448636

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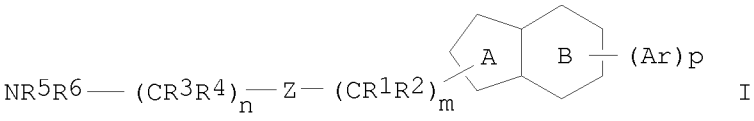


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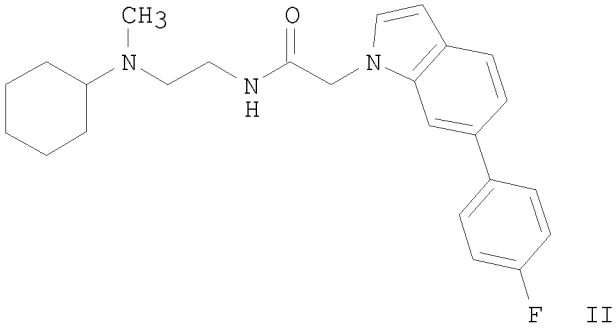


II

AB Title compds. I [wherein R1 - R4 independently = H, halo, alkyl, etc.; R5, R6 independently = H, alkyl, cycloalkyl, etc.; Z = C(O), C(O)O, CONH, etc.; m, n = 1-6; ring A = (un)substituted fused 5-membered heteroaryl or heterocycloalkyl; ring B = (un)substituted fused 6-membered (hetero)aryl or (hetero)cycloalkyl; Ar = (un)substituted (hetero)aryl; p = 0-1] and pharmaceutically acceptable salts, hydrates and N-oxides thereof, which can inhibit the binding of the SDF-1 chemokine to the chemokine receptor CXCR4 and/or the binding of the SDF-1 or I-TAC chemokines to the chemokine receptor CCXCKR2 (CXCR7), were prepared For instance, II was synthesized and had IC50 < 1 μM for both CXCR4 and CXCR7 receptors in chemotaxis or binding assays. The invented compds. and their pharmaceutical compns. are useful for the treatment of CXCR4-mediated diseases or conditions.

L4 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:703476 HCAPLUS
DOCUMENT NUMBER: 147:118229
TITLE: Benzimidazole compounds and their preparation, pharmaceutical compositions and use in the treatment of VR1-mediated diseases
INVENTOR(S): Besidski, Yevgeni; Griffin, Andrew; Labrecque, Denis; Johnstone, Shawn; Jones, Paul; Kers, Inger; Nyloef, Martin; Skogholm, Karin
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 89pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2007073303 | A2 | 20070628 | WO 2006-SE1467 | 20061221 |
| WO 2007073303 | A3 | 20070830 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

| | | | | | |
|---|---|---|---|---|---|
| AU 2006327320 | A1 | 20070628 | AU 2006-327320 | | 20061221 |
| CA 2634804 | A1 | 20070628 | CA 2006-2634804 | | 20061221 |
| US 20080171770 | A1 | 20080717 | US 2006-614346 | | 20061221 |
| EP 1966156 | A2 | 20080910 | EP 2006-835882 | | 20061221 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS | | | | | |
| IN 2008DN05119 | A | 20080926 | IN 2008-DN5119 | | 20080613 |
| MX 2008007837 | A | 20080626 | MX 2008-7837 | | 20080617 |
| KR 2008080212 | A | 20080902 | KR 2008-717908 | | 20080722 |
| NO 2008003246 | A | 20080911 | NO 2008-3246 | | 20080722 |
| CN 101389610 | A | 20090318 | CN 2006-80053368 | | 20080825 |
| PRIORITY APPLN. INFO.: | | | US 2005-753604P | P | 20051223 |
| | | | WO 2006-SE1467 | W | 20061221 |

OTHER SOURCE(S): MARPAT 147:118229
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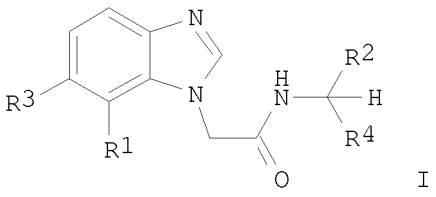


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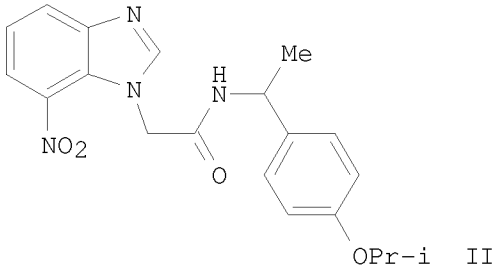


II

AB The invention relates to new compds. formula I or salts, solvates or solvated salts thereof, processes for their preparation and to intermediates used in the preparation thereof, pharmaceutical compns. containing said compds. and to the use of said compds. in therapy. Compds. of formula II wherein R1 is NO2, CN, halo, and acetyl; R2 is (un)substituted Ph, (un)substituted

heteroaryl, (un)substituted PhCH2, and (un)substituted PhOCH2; R3 is H and F; R4 is Me, MeOCO, and Et; R2R4 taken together may form (mono/bi)cyclic ring; and their salts, solvates and solvated salts thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their VR1 inhibitory activity.

L4 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:48925 HCAPLUS
DOCUMENT NUMBER: 146:308386
TITLE: In Silico Binding Free Energy Predictability by Using the Linear Interaction Energy (LIE) Method: Bromobenzimidazole CK2 Inhibitors as a Case Study
AUTHOR(S): Bortolato, A.; Moro, S.
CORPORATE SOURCE: Molecular Modeling Section, Department of Pharmaceutical Sciences, University of Padova, Padua, I-35131, Italy
SOURCE: Journal of Chemical Information and Modeling (2007), 47(2), 572-582
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Protein kinase CK2 is essential for cell viability, and its control regards a broad series of cellular events such as gene expression, RNA, and protein synthesis. Evidence of its involvement in tumor development and viral replication indicates CK2 as a potential target of antineoplastic and antiviral drugs. In this study the Linear Interaction Energy (LIE) Method with the Surface Generalized Born (SGB) continuum solvation model was used to study several bromobenzimidazole CK2 inhibitors. This methodol., developed by Aqvist, finds a plausible compromise between accuracy and computational speed in evaluating binding free energy (ΔGbind) values. In this study, two different free binding energy models, named "CK2scoreA" and "CK2scoreB", were developed using 22 inhibitors as the training set in a stepwise approach useful to appropriately select both the tautomeric form and the starting binding position of each inhibitor. Both models are statistically acceptable. Indeed, the better one is characterized by a correlation coefficient (r2) of 0.81, and the predictive accuracy was 0.65 kcal/mol. The corresponding validation, using an external test set of 16 analogs, showed a correlation coefficient (q2) of 0.68 and a prediction root-mean-square error of 0.78 kcal/mol. In this case, the LIE approach has been proved to be an efficient methodol. to rationalize the difference of activity, the key interactions, and the different possible binding modes of this specific class of potent CK2 inhibitors.
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:298140 HCAPLUS
DOCUMENT NUMBER: 144:331439
TITLE: Preparation of benzimidazol-1-yl-substituted alkanoic acid amides as vanilloid receptor 1 antagonists with analgesic and other therapeutic potential
INVENTOR(S): Besidski, Yevgeni; Kers, Inger; Nyloef, Martin; Slaitas, Andis
PATENT ASSIGNEE(S): AstraZeneca AB, Swed.

SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2006033620 | A1 | 20060330 | WO 2005-SE1364 | 20050919 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| AU 2005285656 | A1 | 20060330 | AU 2005-285656 | 20050919 |
| CA 2577818 | A1 | 20060330 | CA 2005-2577818 | 20050919 |
| EP 1797067 | A1 | 20070620 | EP 2005-783773 | 20050919 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR | | | | |
| CN 101023071 | A | 20070822 | CN 2005-80031737 | 20050919 |
| JP 2008513443 | T | 20080501 | JP 2007-532288 | 20050919 |
| BR 2005015429 | A | 20080722 | BR 2005-15429 | 20050919 |
| IN 2007DN01584 | A | 20070803 | IN 2007-DN1584 | 20070227 |
| MX 2007003119 | A | 20070524 | MX 2007-3119 | 20070315 |
| US 20080015222 | A1 | 20080117 | US 2007-575635 | 20070320 |
| KR 2007056104 | A | 20070531 | KR 2007-706447 | 20070321 |
| NO 2007002005 | A | 20070615 | NO 2007-2005 | 20070419 |

PRIORITY APPLN. INFO.: SE 2004-2284 A 20040921
WO 2005-SE1364 W 20050919

OTHER SOURCE(S): CASREACT 144:331439; MARPAT 144:331439

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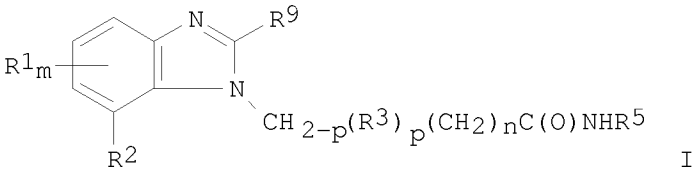

I

AB The present invention relates to benzimidazol-1-yl-substituted alkanoic acid amides (shown as I; variables defined below; e.g. 2-(7-amino-1H-benzimidazol-1-yl)-N-(4-tert-butylbenzyl)acetamide (II)) or salts, solvates or solvated salts thereof, processes for their preparation and to new intermediates used in the preparation thereof, pharmaceutical compns. containing said compds. and to the use of said compds. in therapy. For I: R1 is H, NO2, halo, NR6R7, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6

haloalkyl, C1-6 haloalkyl O, R6OC0-6 alkyl, R6CO, R6OCO, or CONR6R7; m = 0-3; R2 is H, NO2, halo, NR6R7, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 haloalkyl, C1-6 haloalkyl O, cyano, R6OC0-6 alkyl, R6CO, R6OCO, R6CONR7, R6R7NCO, R8SO2, R8SO2HN, aryl C0-6 alkyl or heteroaryl C0-6 alkyl; R3 and R9 = H or C1-4 alkyl; R2 and R3 optionally form a ring; p = 0-2; n = 0, 2, 3, or 4; R5 is C1-10 alkyl, C6-10 aryl C0-6 alkyl, C3-7 cycloalkyl C0-6 alkyl, or C5-6 heteroaryl C0-6 alkyl, whereby any aryl, heteroaryl,or cycloalkyl may be fused with aryl, heteroaryl, C3-7 cycloalkyl, or C3-7 heterocycloalkyl, and which R5 may be substituted with ≥1 A; A is H, OH, NO2, cyano, R6CO, R6O(CO), halo, C1-6 alkyl, NR6R7, C1-6 haloalkyl, C1-6 haloalkyl O, R6OC0-6 alkyl, hydroxy C1-6 alkyl, R8SO2, R8SO2HN, C5-6 aryl O or CONR6R7; R6 and R7 = H or C1-6 alkyl; and R8 is NR6R7 or C1-4 alkyl. Although the methods of preparation are not claimed, prepns. and/or characterization data for 65 examples of I are included. Many of the examples were prepared from a 7-substituted (1H-benzimidazol-1-yl)acetic acid (prepns. described) and an amine in MeCN in the presence of Et3N and O-(7-azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate. IC50 values for 4 examples of I acting as antagonists of the vanilloid receptor 1 in the presence of agonists like capsaicin or 2-(morpholino)ethanesulfonic acid are tabulated.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:103871 HCAPLUS
DOCUMENT NUMBER: 144:192238
TITLE: Preparation of N-(4-sulfamoylphenyl) amides as inhibitors of voltage-gated sodium channels
INVENTOR(S): Gonzalez, Jesus E.; Termin, Andreas P.; Martinborough, Esther; Zimmerman, Nicole
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 353 pp., Cont.-in-part of U.S. Ser. No. 914,988.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| US 20060025415 | A1 | 20060202 | US 2005-60719 | | 20050217 |
| US 20050137190 | A1 | 20050623 | US 2004-914988 | | 20040809 |
| PRIORITY APPLN. INFO.: | | | US 2003-493659P | P | 20030808 |
| | | | US 2004-584717P | P | 20040704 |
| | | | US 2004-914988 | A2 | 20040809 |

OTHER SOURCE(S): CASREACT 144:192238; MARPAT 144:192238
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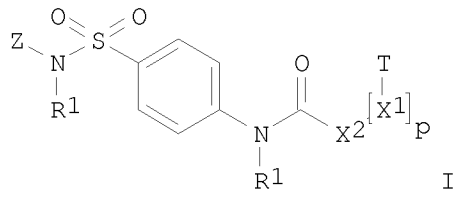

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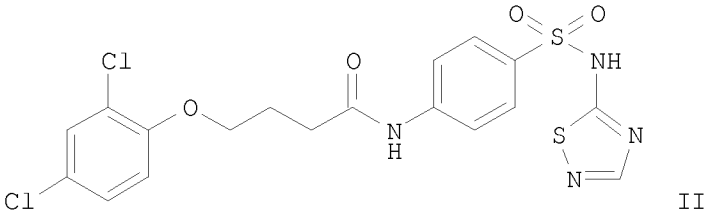

II

AB The title compds. I [R1 = H, (un)substituted alkyl; X1 = O, S, (un)substituted NH; p = 0-1; X2 = (un)substituted alkylene; Z = thiazolyl, imidazolyl, oxazolyl, etc.; T = (un)substituted Ph, 8-14 membered (non)aromatic bicyclic or tricyclic ring having 0-5 heteroatoms selected from O, S, N, NH, SO, SO2, etc.], useful as inhibitors of voltage-gated sodium channels, were prepared E.g., a multi-step synthesis of II, starting from 2,4-dichlorophenol and Et 4-bromobutyrate, was given. The compds. I were found to inhibit voltage-gated sodium channels at 25.0 μM or less. I were also found possess desired N-type calcium channel modulation activity and selectivity (no data given). The invention also provides pharmaceutically acceptable compns. comprising the compds. I and methods of using the compns. in the treatment of various disorders.

L4 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103734 HCAPLUS
DOCUMENT NUMBER: 143:386764
TITLE: Preparation of aniline derivatives as kininogenase inhibitors
INVENTOR(S): Tokumasu, Munetaka; Sugiki, Masayuki; Hirashima, Haruko; Matsumoto, Hideki; Yoshimura, Toshihiko; Nogi, Yasuko; Takahashi, Mitsuo; Kitazawa, Manabu; Oonuki, Akiko; Fukuchi, Naoyuki; Shima, Yoichiro
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan; et al.
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005095327 | A1 | 20051013 | WO 2005-JP6834 | 20050331 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

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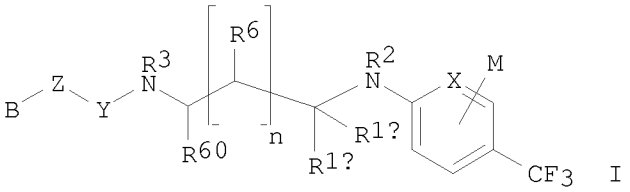
|---|---|---|---|---|
| EP 1736465 | A1 | 20061227 | EP 2005-728768 | 20050331 |
| US 20070066586 | A1 | 20070322 | US 2006-537139 | 20060929 |

PRIORITY APPLN. INFO.: JP 2004-107368 A 20040331
WO 2005-JP6834 W 20050331

OTHER SOURCE(S): MARPAT 143:386764
GI



AB The title compds., e.g. I [X = C, N ; M = H, halo, (un)substituted alkyl, etc.; Z = single bond, CH:CH, CO, etc.; B = H, (un)substituted alkyl, etc.; R3 = H, (un)substituted alkyl, (un)substituted aryl; further detail on R3 is given; Y = CO, SO2; R1a, R1b = H, (un)substituted alkyl, (un)substituted aryl; further detail on R1a and R1b is given; R2 = H, alkyl; further detail related to R1a, R1b and R2 is given; n = 0 or 1; R6 and R60 = H, (un)substituted alkyl, amino, etc.], are prepared Thus, N-((2R)-3-methyl-2-[[4-(trifluoromethyl)phenyl]-amino]butyl)-2-phenylacetamide CF3CO2H salt was prepared in 3 steps from 4-trifluoromethyliodobenzene and D-valine. In an in vitro test for tissue kallikrein inhibiting activity, compds. of this invention showed pIC50 values of 6.51 to 7.70. In a test for analgesic activity using mice, compds. of this invention at 30 mg/kg orally showed activity equal to that of indomethacin at 10 mg/kg orally.

L4 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:1019865 HCAPLUS
DOCUMENT NUMBER: 142:6536
TITLE: A preparation of benzimidazole derivatives, useful as inhibitors of vanilloid receptor 1
INVENTOR(S): Besidski, Yevgeni; Kers, Inger; Nyloef, Martin; Rotticci, Didier; Slaitas, Andis; Svensson, Mats
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004100865 | A2 | 20041125 | WO 2004-SE738 | 20040513 |
| WO 2004100865 | A3 | 20050120 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2004238177 | A1 | 20041125 | AU 2004-238177 | 20040513 |
| AU 2004238177 | B2 | 20080424 | | |
| CA 2525628 | A1 | 20041125 | CA 2004-2525628 | 20040513 |
| EP 1626964 | A2 | 20060222 | EP 2004-732865 | 20040513 |
| EP 1626964 | B1 | 20090121 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR | | | | |
| BR 2004010316 | A | 20060523 | BR 2004-10316 | 20040513 |
| CN 1784387 | A | 20060607 | CN 2004-80012619 | 20040513 |
| CN 100413849 | C | 20080827 | | |
| JP 2006528971 | T | 20061228 | JP 2006-532186 | 20040513 |
| RU 2337098 | C2 | 20081027 | RU 2005-136529 | 20040513 |
| CN 101328150 | A | 20081224 | CN 2008-10136051 | 20040513 |
| AT 421506 | T | 20090215 | AT 2004-732865 | 20040513 |
| IN 2005DN04859 | A | 20071012 | IN 2005-DN4859 | 20051024 |
| US 20060287377 | A1 | 20061221 | US 2005-556229 | 20051109 |
| MX 2005012247 | A | 20060210 | MX 2005-12247 | 20051114 |
| NO 2005005977 | A | 20060216 | NO 2005-5977 | 20051215 |
| AU 2008203305 | A1 | 20080814 | AU 2008-203305 | 20080724 |
| PRIORITY APPLN. INFO.: | | | SE 2003-1446 A | 20030516 |
| | | | SE 2004-43 A | 20040112 |
| | | | AU 2004-238177 A3 | 20040513 |
| | | | CN 2004-80012619 A3 | 20040513 |
| | | | WO 2004-SE738 W | 20040513 |
| OTHER SOURCE(S): | MARPAT 142:6536 | | | |

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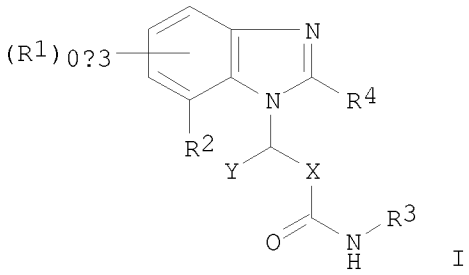

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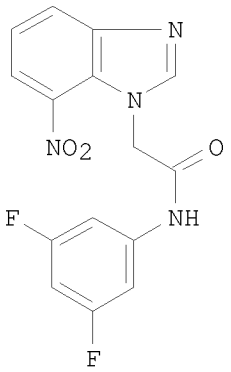

II

AB The invention relates to a preparation of new benzimidazole derivs. of formula I [wherein: X is CH2 or (CH2)2-4; Y is H or (alkyl)0-2; R1 is H, NO2, halogen, alk(en/yn)yl, or (H/alkyl)C(O), etc.; R2 is NO2, halogen, alk(en/yn)yl, or haloalkyl, etc.; R3 is alkyl, arylalkyl, cycloalkylalkyl, or heteroarylalkyl, etc.; R4 is H or alkyl], useful as inhibitors of vanilloid receptor 1 (VR 1). For instance, benzimidazole derivative II was prepared via amidation of 2-(7-nitro-1H-benzimidazol-1-yl)acetic acid by 3,5-difluoroaniline. The prepared title compds. were screened in fluorometric image plate reader assay (hVR1 FLIPR) (II, IC50 = 50 nM).
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:920737 HCAPLUS
DOCUMENT NUMBER: 142:247
TITLE: Optimization of Protein Kinase CK2 Inhibitors Derived from 4,5,6,7-Tetrabromobenzimidazole
AUTHOR(S): Pagano, Mario A.; Andrzejewska, Mariola; Ruzzene, Maria; Sarno, Stefania; Cesaro, Luca; Bain, Jenny; Elliott, Matthew; Meggio, Flavio; Kazimierczuk, Zygmunt; Pinna, Lorenzo A.
CORPORATE SOURCE: Dipartimento di Chimica Biologica, Universita di Padova, Padua, Italy
SOURCE: Journal of Medicinal Chemistry (2004), 47(25), 6239-6247
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:247

AB Casein kinase 2 (CK2) is a ubiquitous, essential, and highly pleiotropic protein kinase whose abnormally high constitutive activity is suspected to underlie its pathogenic potential in neoplasia and infective diseases. Thus, CK2 inhibitors designed to dissect the signaling pathways affected by this kinase, in perspective, may give rise to pharmacol. tools. One of the most successful CK2 inhibitors is TBB (4,5,6,7-tetrabromobenzotriazole). Here we show that its inhibitory properties can be markedly improved by generating adducts in which N2 is replaced by a carbon atom bound to a variety of polar functions. The most efficient inhibitor is 4,5,6,7-tetrabromo-2-(dimethylamino)benzimidazole (2c) followed by the methylsulfanyl (8), isopropylamino (2e), and amino (2a) congeners. All these compds. display Ki values <100 nM (40 nM in the case of 2c). 2C induces apoptosis of Jurkat cells more readily than TBB (DC50 value 2.7 vs 17 μM) and, unlike TBB, it does not display any side effect on mitochondria polarization up to 10 μM concentration Mol. modeling of the CK2-2c complex, based on the crystal structure of the CK2-TBB complex suggests that a number of addnl. apolar contacts between its two Me groups and hydrophobic residues nearby could account for its superior inhibitory properties. Consequently, 2c is even more susceptible than TBB to mutations of the unique hydrophobic residues V66 and/or I174 to alanine. We propose to adopt 2c as first choice CK2 inhibitor instead of TBB, especially for in cell studies.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:219222 HCAPLUS

DOCUMENT NUMBER: 132:222537

TITLE: Preparation of substituted nitrogen-containing heterocyclic compounds

INVENTOR(S): Horvath, Andras; Salamon, Zoltan

PATENT ASSIGNEE(S): Hung.

SOURCE: Hung. Teljes, 21 pp.
CODEN: HUXXBU

DOCUMENT TYPE: Patent

LANGUAGE: Hungarian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| HU 78019 | A2 | 19990528 | HU 1995-962 | 19950331 |

PRIORITY APPLN. INFO.: HU 1995-962 19950331

OTHER SOURCE(S): MARPAT 132:222537

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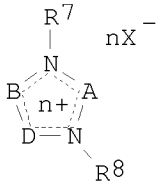


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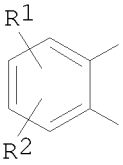


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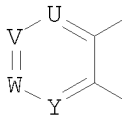


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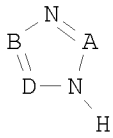
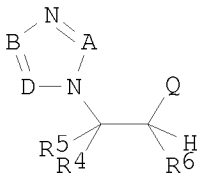



IV




V

AB The title compds. [I; A = CR1, CR3; B = CR1; D = CR2, CR2:CR3, N; BD = II, III; R1-R3 = H, alkyl; U, V, W, Y, Z = (un)substituted Ph, NHCOalkyl, CO2alkyl, etc.; n = 0-1; X = Cl, Br, I, etc.; R7 = H, alkyl, heteroaryl; R8 = H, CR4R5CHR6Q; R4-R6 = H, alkyl, cycloalkyl, Q; Q = CN, CO2alkyl, COalkyl, etc.], useful as intermediates for biol. active compds., were prepared by reacting compound IV with olefin R4R5C:CR6Q followed by treatment of N-monoalkylated compound V with R7X.

L4 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:866656 HCAPLUS
DOCUMENT NUMBER: 124:117179
ORIGINAL REFERENCE NO.: 124:21829a,21832a
TITLE: Michael adducts in the regioselective synthesis of N-substituted azoles
AUTHOR(S): Horvath, Andras
CORPORATE SOURCE: Alkaloida Chem. Co. Ltd., Tiszavasvari, Hung.
SOURCE: Synthesis (1995), (9), 1183-9
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:117179
AB Michael adducts of azoles (4-phenyl-, 4-methyl-, and 4-nitroimidazole, 4-methylbenzimidazole, 1,2,4-triazole, and theophylline) are shown to be valuable substrates for obtaining the N-substituted derivs. of the parent heterocycles by a quaternization-Hofmann elimination sequence. The effectiveness of the procedure is dependent on the regiochem. outcome of the 1st, N-protective step, i.e. the Michael addition By choosing the appropriate Michael acceptor, alkylating agent, and deprotection conditions, the thermodynamically less stable regioisomers of N-substituted azoles were obtained in high yields.

L4 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:510007 HCAPLUS
DOCUMENT NUMBER: 97:110007
ORIGINAL REFERENCE NO.: 97:18305a,18308a

TITLE: Benzimidazoles
INVENTOR(S): Jemison, Robert William; Beames, David John
PATENT ASSIGNEE(S): ICI Australia Ltd. , Australia
SOURCE: Pat. Specif. (Aust.), 56 pp.
CODEN: ALXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| AU 519236 | B2 | 19811119 | AU 1978-35043 | 19770422 |
| AU 7835043 | A | 19791018 | | |

PRIORITY APPLN. INFO.: AU 1977-9860 A 19770422
OTHER SOURCE(S): CASREACT 97:110007
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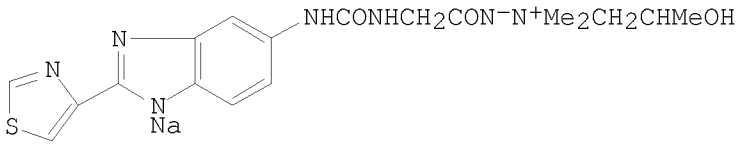


I

AB R[XN-N+R1R2R3]n [R = (un)substituted benzimidazolyl, R1-R3 = (un)substituted alkyl; X = CO, O2C, NHCO, X1CO, COX1CO, NHCOX1CO, CONHX1CO, SO2, 4-SC6H4O2C, NHCONHX1CO, 4-COC6H4O2C, 4-COC6H4NHCO, 4-SOC6H4CO, 4-COC6H4CO, 4-SOC6H4O2C; X1 = alkylene; n = 1-3] were prepared Thus 5-amino-2-(4-thiazolyl)benzimidazole was treated with OCNCH2CO2Me to give the 5-methoxycarbonylmethylureidobenzimidazole derivative which was treated with Me2NNH2 and propylene oxide to give I. At 50 mg/kg s.c. in sheep I reduced the fecal Hemonchus egg count from 800 to 0 on the 2nd day.

L4 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:88247 HCAPLUS
DOCUMENT NUMBER: 70:88247
ORIGINAL REFERENCE NO.: 70:16521a,16524a
TITLE: Participation of the anilino group in peptide bond cleavage. Use of tert-butyl 3,5-dinitro-2-fluorocarbanilate as a peptide reagent
AUTHOR(S): Kirk, Kenneth L.; Cohen, Louis A.
CORPORATE SOURCE: Nat. Inst. of Allergy and Metab. Diseases, Nat. Inst. of Health, Bethesda, MD, USA
SOURCE: Journal of Organic Chemistry (1969), 34(2), 395-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Picramyl fluoride (3,5-dinitro-2-fluoroaniline) (I) was prepared by the SnCl2 reduction of picryl fluoride and by the Curtius rearrangement of 3,5-dinitro-2-fluorobenzoyl azide. Reaction of I with peptides (at pH 8) results in replacement of the F atom by the peptide N. Coupling is followed by rapid intramol. attack of the anilino group on the neighboring peptide bond (even at pH 8), resulting in cleavage of that bond and the

formation of a dihydro-quinoxalinone derivative of the N-terminal amino acid. By use of I tert-BuO2C derivative, the coupling and cleavage steps can be separated Removal of the blocking group by F3CCO2H is followed by rapid cyclization, both reactions proceeding quant. Sequencing of a polypeptide (e.g., oxidized insulin A chain) provides steadily decreasing yields of N-terminal derivs., due to benzimidazolinone formation during the coupling step. By kinetic anal., it is shown that the benzimidazolinone arises from attack of the 2,4-dinitroaniline anion on the adjacent tert-Bu carbanilate group.

=> log y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 87.51 | 273.61 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -15.58 | -15.58 |

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